Program of 7th ForMGE
Opening Ceremony & Plenary Session

Date: Dec 6th 2023 (Beijing time, UTC+8) **Venue: Changjiang Grand Hall, 1st floor, Shancheng International Conference Center, Chongqing**

Opening Ceremony		
Chair: Prof. Pan Fusheng, Academician of CAE		
O1	8:45-10:25	Guests Introduction
		Opening and Welcome Remarks
O2		MGE Outstanding Achievement and Contribution Award Ceremony
O3		MGE Young Scientist Award Ceremony
O4		Journal Launch Ceremony of "*Materials Genome Engineering Advances*"
O5		Introduction of Western China (Chongqing) Science City and Projects Signing Ceremony

Plenary Speech				
No.	**Time**	**Speaker**	**Affiliations**	**Presentation Title**
Session Chair: Prof. Han En-Hou, Academician of CAE; Prof. Zhang Fucheng, Academician of CAE				
P1-01	10:25-11:00	Prof. Chen Liquan	Institute of Physics CAS, Academician of CAE	Material Systems Engineering, Boosting the Leadership in Lithium Battery Field
P1-02	11:00-11:35	Prof. Wang Haizhou	China Iron & Steel Research Institute Group, Academician of CAE	High-throughput statistical mapping for reverse engineering research and its application in engineering materials
P1-03	11:35-12:10	Prof. Shyue Ping Ong	University of California, San Diego, U.S.	Materials Design at Scale with Universal Machine Learning Models and Big Data

	12:10-13:30	Lunch		
Session Chair: Prof. Liu Riping, Academician of CAE; Prof Jiang Chengbao, Academician of CAS				
P1-04	13:30-14:05	Prof. Wang Yuzhong	Sichuan University, Academician of CAE	The Constructed Contribution Model between Motif Structure and Flame Retardance Originated from Real Burning Big Data toward Fire-Proof Polymeric Materials Design
P1-05	14:05-14:40	Prof. E Weinan	Peking University, Academician of CAE	Pre-trained models in materials science
P1-06	14:40-15:15	Prof. Turab Lookman	AiMaterials Research LLC, U.S.	The Importance of Sequential Design in Materials Discovery
	15:15-15:30	Tea Break		
Session Chair: Prof. Zhao Zhongwei, Academician of CAE; Prof Chen Lidong, Academician of CAS				
P1-07	15:30-16:05	Prof. Wang Yunzhi	Ohio State University, U.S.	Integrated Computational Engineering of Compositionally and Structurally Modulated Materials
P1-08	16:05-16:40	Prof. Huang Xiaoxu	Chongqing University, China	Three-dimensional orientation reconstruction and high-throughput characterization of polycrystalline material structural parameters
P1-09	16:40-17:15	Prof. Woo jin Choi	The Korea Research Institute of Chemical Technology, Korea	Materials Data Standardization for AI-ready Data in Korea
Poster, Exhibition and Banquet				

Technical Symposia

Symposia 1: High-Efficiency Materials Computation and Design

Symposium Organizers: Yang Mingli, Sichuan University; Sun Zhimei, Beihang University; Yuan Yuan, Chongqing University; Zhao Yuhong, University of Science and Technology Beijing; Miao Naihua, Beihang University

Date: Dec 7th 2023 (Beijing time, UTC+8) **Venue: Jialing-1 Hall, 2nd floor, Shancheng International Conference Center, Chongqing**

No.	Time	Speaker	Affiliations	Presentation Title
Session Chair: Song Haifeng, Institute of Applied Physics and Computational Mathematics; Yuan Yuan, Chongqing University				
S1-01	8:30-8:55	Li Shuhua	Nanjing University	Linear scaling quantum chemistry methods for material systems
S1-02	8:55-9:20	Wang Linwang	Institute of Semiconductors	First principles material simulation software development for industry
S1-03	9:20-9:45	Cheng Xingwang	Beijing Institute of Technology	ICME-aided design of novel titanium alloys for warhead
S1-04	9:45-10:10	Ouyang Chuying	CATL (Contemporary Amperex Technology Co., Limited)	Computing and data-driven research and development for new energy battery materials—Material genetic engineering empowers industrial innovation
	10:10-10:20	Tea Break		
Session Chair: Cheng Xingwang, Beijing Institute of Technology; Yang Mingli, Sichuan University				
S1-05	10:20-10:45	Song Haifeng	Institute of Applied Physics and Computational Mathematics	Progress of ProMe, an integrated computing platform for physical properties of extreme materials
S1-06	10:45-11:10	Zhang Chaoyang	Institute of Chemical Materials, CAEP	Progress in Intelligently Designing Energetic Molecules
S1-07	11:10-11:35	Sun Zhimei	Beihang University	Graph Convolutional Machine Learning Potential for Sb-Te Binary Compounds of Multiple Stoichiometries
S1-08	11:35-12:00	Zhang Linfeng	DP Technology	AI-Assisted Material R&D: From Multiscale to Pre-trained Models (Awarded Lecture)
	12:00-13:30	Lunch		

Session Chair: Sun Zhimei, Beihang University; Zhao Yuhong, University of Science and Technology Beijing				
S1-09	13:30-13:55	Chang Keke	Ningbo Institute of Materials Technology and Engineering, CAS	Data-Driven Design of Structure and Properties for Cermet
S1-10	13:55-14:20	Wang Junsheng	Beijing Institute of Technology	Al-Li alloy by design via integrating in-situ SANS measured and DFT predicted kinetics
S1-11	14:20-14:45	Liu Sida	Xi'an Jiaotong University	Design and Toughening of High-performance Alloy Coatings and Heat-resistant Aluminum Alloys based on Theoretical Calculations
S1-12	14:45-15:10	ZHANG Shangzhou	Yantai University/Institute of Metal Research, CAS	First-principles investigations of the interaction between alloying atom and dislocation and its implication to the rafting of Ni-based superalloys
S1-13	15:10-15:35	Jin Jianfeng	Northeastern University	Multiscale simulation on recrystallization texture and bimodal microstructure towards high-strength/plasticity of wrought magnesium alloy
	15:35-15:50	Tea Break		
Session Chair: Miao Naihua, Beihang University; Xu Dingguo, Sichuan University				
S1-14	15:50-16:15	Yuan Yuan	Chongqing University	The multi-solute solid solution cocktail-effects of magnesium alloys and their application on materials design
S1-15	16:15-16:40	Yang Jiong	Shanghai University	High-Throughput Calculations for Thermoelectrics Based on MatHub-3d Repository
S1-16	16:40-17:05	Zhang Xie	Northwestern Polytechnical University	High-Throughput Computational Design of Deep-Ultraviolet Light Emitters
S1-17	17:05-17:30	Lu Hao	Beijing University of Technology	Design of Cemented Carbides Based on Multiscale Modeling
S1-18	17:30-17:55	Hu Ruiqin	Dassault Systèmes (Shanghai)	V+R Generative Materials Design by Dassault Systèmes

Symposium 2: Revolutionary Materials Experimental Technology

Symposium Organizers: Liu Zhifu, Shanghai Institute of Ceramics, CAS; Huang Xiaoxu, Chongqing University; Zhou Kechao, Central South University; Yang Zhongmin, South China Normal University; Zhang Peng, Shanghai Jiao Tong University; Dong Guoping, South China University of Technology; Wang Zegao, Sichuan University

Date: Dec 7th 2023 (Beijing time, UTC+8) **Venue: Gele Hall, 2nd floor, Shancheng International Conference Center, Chongqing**

No.	Time	Speaker	Affiliations	Presentation Title
Session Chair: Zhang Peng, Shanghai Jiao Tong University; Guo Yueling, Beijing Institute of Technology				
S2-01	8:30-8:55	Wang Hong	Shanghai Jiao Tong University	Data Factory – Transformative materials data generation infrastructure
S2-02	8:55-9:20	Su Hang	China Iron and Steel Research Institute Group	The "Unmanned Data Factory" for Metal Structural Materials
S2-03	9:20-9:45	Zhou Xiaoyuan	Chongqing University	Strategies towards high mobility in thermoelectric materials
S2-04	9:45-10:10	Deng Lu	Shanghai Institute of Optics and Fine Mechanics, CAS	Machine learning driven method of designing new glass materials
S2-05	10:10-10:35	Wang Zhilei	University of Science and Technology Beijing	Current situation and thinking regarding the key technology of materials digital twining
	10:35-10:50	Tea Break		
Session Chair: Dong Guoping, South China University of Technology; Wang Zhilei, University of Science and Technology Beijing				
S2-06	10:50-11:20	Sun Yong	Beijing Mechanical and Electrical Research Institute, China Machinery General Institute Group	Research on traceability quality control technology of the whole process of plastic forming of precision forgings
S2-07	11:20-11:55	Liu Yi	Shanghai University	Thousand-level high-throughput experiment and machine learning optimization of composition and processing of high-strength and high-conductivity cooper alloys
S2-08	11:55-12:05	Deng Lei	Huazhong University of Science and Technology	Intelligent online detection and simulation of titanium alloy deformation state for forging digital twin system
S2-09	12:05-12:30	Guo Yueling	Beijing Institute of Technology	Multi-wire and multi-arc parallel additive manufacturing technology and material/structure high-throughput fabrication (Awarded Lecture)
	12:30-13:30	Lunch		

Session Chair: Liu Yi, Shanghai University; Xu Jiazhuang, Sichuan University				
S2-10	13:30-13:55	Chen Houwen	Chongqing University	Simultaneous characterization of structure and composition of precipitates in light alloys
S2-11	13:55-14:20	Xu Jiazhuang	Sichuan University	The construction of synchrotron radiation high- throughput characterization device for polymer injection molding and its in-situ study on structure manipulation (Awarded Lecture)
S2-12	14:20-14:45	Gao Meng	Ningbo Institute of Materials Technology and Engineering, CAS	High-throughput screening of physical and chemical properties of new metal materials
S2-13	14:45-15:10	Wang Yongzhe	Shanghai Institute of Ceramics, CAS	On-axis TKD patterns indexing with two-step correlation and TKD-Unet model
S2-14	15:10-15:35	Luo Jinru	Suzhou Laboratory	Design and Manufacture of the ODS-steel with high strength and ductility by a high-throughput preparation method
	15:35-15:50	Tea Break		
Session Chair: Liu Zhifu, Shanghai Institute of Ceramics, CAS; Wang Zegao, Sichuan University				
S2-15	15:50-16:15	Bai Yang	University of Science and Technology Beijing	Autonomous experimental system of function ceramics
S2-16	16:15-16:40	Zhao Yicheng	University of Electronic Science and Technology of China	From Liquids to Electronics: A High-Throughput Intelligent Experimental Platform
S2-17	16:40-17:05	Huijian	Shanghai Jiao Tong University	A high-throughput experimental data-driven platform for the development of new materials (Awarded Lecture)
S2-18	17:05-17:30	Jiang Jing	Zhejiang Lab	Gas sensor and heterogeneous array optimization by a robotic platform

Symposium 3: Materials Big Data and Intelligent Technologies

Symposium Organizers: Su Yanjing, University of Science and Technology Beijing; Wang Hong, Shanghai Jiao Tong University; Xue Dezhen, Xi'an Jiaotong University; Huang Weijiu, Chongqing University of Arts and Sciences; Wang Yi, Northwestern Polytechnical University; Fu Huadong, University of Science and Technology Beijing

Date: Dec 7th 2023 (Beijing time, UTC+8) **Venue: Jialing Hall-2, 2nd floor, Shancheng International Conference Center, Chongqing**

No.	Time	Speaker	Affiliations	Presentation Title
Session Chair: Liu Jianjun, Shanghai Institute of Ceramics, CAS; Wang Yi, Northwestern Polytechnical University				
S3-01	8:30-8:55	Liu Jianjun	Shanghai Institute of Ceramics, CAS	A data-driven intelligent research and development system for ceramic materials
S3-02	8:55-9:20	Yu Fan	Huawei Technologies Co., Ltd.	Trends in AI Scientific Computing and MindSpore Practice
S3-03	9:20-9:45	Zhang Lijun	Central South University	High-performance alloy design driven by a combination of computational thermodynamics/kinetics and machine learning
S3-04	9:45-10:10	Yuan Ruihao	Northwestern Polytechnical University	Enhancing prediction of alloys property using pre-trained model (Awarded Lecture)
	10:10-10:20	Tea Break		
Session Chair: Wang Hong, Shanghai Jiao Tong University; Yin Haiqing, University of Science and Technology Beijing				
S3-05	10:20-10:45	Yin Haiqing	University of Science and Technology Beijing	Composition optimization of nickel-based superalloys with γ'+γ" precipitation phases and ML modeling of thermal deformation behavior
S3-06	10:45-11:10	Chen Xiang	Tsinghua University	Artificial Intelligence Design of Lithium Battery Electrolytes
S3-07	11:10-11:35	Liu Xinyan	University of Electronic Science and Technology of China	Machine learning-aided design for energy materials and devices
S3-08	11:35-12:00	Zhang Lei	Nanjing University of Information Science and Technology	Data-driven prediction and optimization of emerging photovoltaic materials
	12:00-13:30	Lunch		

Session Chair: Fu Huadong, University of Science and Technology Beijing; Chong Xiaoyu, Kunming University Of Science and Technology				
S3-09	13:30-13:55	Chong Xiaoyu	Kunming University Of Science and Technology	Application of the Noble Metal Materials Genome Engineering Database in the Integrated Design of Multiphase Noble Metal Superalloys
S3-10	13:55-14:20	Chen Pin	National Supercomputer Center in Guangzhou	Large-scale Materials Generation Model on Supercomputer: Methods, Principles, and Applications
S3-11	14:20-14:45	Jiang Xue	University of Science and Technology Beijing	Exploring the application of natural language processing in materials (Awarded Lecture)
S3-12	14:45-15:10	Xu Ben	China Academy of Engineering Physics	Atomic Potential for Magnetic Materials
	15:10-15:20	Tea Break		
Session Chair: Xue Dezhen, Xi'an Jiaotong University; Wang Chenchong, Northeastern University				
S3-13	15:20-15:45	Wang Chenchong	Northeastern University	Predicting the Stress-Strain Behavior Using Deep Learning Based on Crystal Plasticity Theory
S3-14	15:45-16:10	Li Minjie	Shanghai University	Application of Small Sample Machine Learning in Materials Design
S3-15	16:10-16:35	Qiao Haibo	CITIC Dicastal Co., Ltd.	Development of Materials Model for Aluminum Castings Considering Microstructure Inhomogeneity
S3-16	16:35-17:00	Song Ce	Dalian University of Technology	Data-driven Rational Design of High-performance Poly(aryl ether)s

Symposium 4: MGE Technologies and Industrial Application

Symposium Organizers: Xiang Yong, University of Electronic Science and Technology of China; Han En-Hou, Institute of Corrosion Science and Technology; Li Jinshan, Northwestern Polytechnical University; Bai Shuxin, National University of Defense Technology; Chen Xianhua, Chongqing University; Wu Fang, University of Electronic Science and Technology of China; Liu Zhe, Northwestern Polytechnical University; Wang Haitao, Institute of Corrosion Science and Technology; Ye Yichong, National University of Defense Technology; Wang Zhilei, University of Science and Technology Beijing

Date: Dec 7th 2023 (Beijing time, UTC+8) **Venue: Gujian Meeting Room, 3rd floor, Shancheng International Conference Center, Chongqing**

No.	Time	Speaker	Affiliations	Presentation Title
Session Chair: Yang Xiaoyu, Computer Network Information Center, CAS; Chen Xianhua, Chongqing University				
S4-01	8:30-8:55	Du Yong	Central South University	Phase diagram and phase transition software and intelligent design examples of engineering materials
S4-02	8:55-9:20	Zhang Tiantian	Sington Technologies Co., Ltd.	The Boundaries of Computational Simulation Methods in Materials R&D and Development in Manufacturing Application Scenarios
S4-03	9:20-9:45	Chen Xianhua	Chongqing University	Research and Application of Magnesium Alloys for Functional Integration of Material Structures
S4-04	9:45-10:10	Hu Lianglin	Computer Network Information Center, Chinese Academy of Sciences	Challenges and Reflections on Elemental Services for Scientific Data
	10:10-10:20	Tea Break		
Session Chair: Du Yong, Central South University; Wu Fang, University of Electronic Science and Technology of China				
S4-05	10:20-10:45	Liu Yuyang	DeepVerse (Shanghai) LTD	DeepVerse: Materials Informatics for Industrial Applications
S4-06	10:45-11:10	Hu Xiaoran	Chengdu Xinzhao Technology Co., Ltd.	High-throughput preparation, characterization and industrial application of intelligent sensing materials and devices (Awarded Lecture)
S4-07	11:10-11:35	Liu Libin	Central South University	Design of Alloys and Processes with the CALPHAD method
S4-08	11:35-12:00	Zhang Zhi	Central Research Institute, China Baowu Steel Group	On the Development and Application of ICME in HSM Work Rolls
	12:00-13:30	Lunch		

Session Chair: Wang Leyun, Shanghai Jiao Tong University; Liu Zhe, Northwestern Polytechnical University				
S4-09	13:30-13:55	Wang Leyun	Shanghai Jiao Tong University	Reflections and Practices on the Industrial Application of Material Genome Engineering
S4-10	13:55-14:20	Yang Xiaoyu	Computer Network Information Center, CAS	Industrialization of MatCloud High throughput Intelligent Materials Computational Platform: Experiences and Insights
S4-11	14:20-14:45	Han Hao	University of Toronto	Delocalized, Asynchronous, Closed-Loop Discovery of Organic Laser Emitters
S4-12	14:45-15:10	Kong Decai	CITIC Dicastal Co., Ltd	Virtual R&D Technology for Casting Wheels Based on Integrated Computational Materials Engineering
S4-13	15:10-15:35	Yang Li	China Iron & Steel Research Institute Group	Metal Material Digital R&D Platform and Engineering Applications
	15:35-15:50	Tea Break		
Session Chair: Hu Xiaoran, Chengdu Xinzhao Technology Co., Ltd.; Han Hao, University of Toronto				
S4-14	15:50-16:15	Feng Jing	Kunming University of Science and Technology	Development and engineering application of low stress thermal barrier coatings based on multi-scale integrated computing and machine learning (Awarded Lecture)
S4-15	16:15-16:40	Qiu Cheng	Institute of Mechanics , Chinese Academy of Sciences	Data-Driven Applications in Composite Materials Engineering
S4-16	16:40-17:05	Wang Zhuo	Chengdu Caizhi Technology Co., Ltd.	Practice of Material Digital Intelligence Industrial Application Based on Data, Computation and AI
S4-17	17:05-17:30	Ji Chunlin	Kuang-Chi Institute of Advanced Technology	An intelligent research and development platform for multi-objective and collaborative optimization of functional materials
S4-18	17:30-17:55	Wang Yin	Che-Hung Micro Technology (Shanghai) Co., Ltd.	Material Digital R&D Platform Empowering Intelligent Manufacturing

Symposium 5: AI for Material Science — International Track1

Symposium Organizers: Zhang Dawei, University of Science and Technology; Sun Zhimei, Beihang University; Xue Dezhen, Xi'an Jiaotong University; Liu Zhe, Northwestern Polytechnical University; Zhang Peng, Shanghai Jiao Tong University; Feng Qiang, University of Science and Technology; Zhou Xiaoyuan, Chongqing University; Zhang Xiaokun, University of Electronic Science and Technology of China

Date: Dec 7th 2023 (Beijing time, UTC+8) **Venue: Zhongliang Hall, 2nd floor, Shancheng International Conference Center, Chongqing**

No.	Time	Speaker	Affiliations	Presentation Title
Session Chair: Sun Zhimei, Beihang University				
I5-01	8:30-9:00	Han Seungwu	Seoul National University	Material discovery and process simulation by machine learning potential
I5-02	9:00-9:30	Sun Ziqi	Queensland University of Technology	Rational design of 2D nanomaterials for sustainable energy storage and conversion
I5-03	9:30-10:00	Mo Yifei	University of Maryland, College Park	Accelerated Computational Materials Design for Next-Generation Batteries
	10:00-10:15	Tea Break		
Session Chair: Zhang Wei, Xi`an Jiaotong University				
I5-04	10:15-10:45	Li Ning	South China University of Technology	Materials Genome Engineering Accelerates the Research and Development of Organic Optoelectronic Technologies (Awarded Lecture)
I5-05	10:45-11:15	Ling Chen	Toyota Motor North America	Materials informatics in industrial applications: from fundamentals to device design and monitoring
I5-06	11:15-11:45	Zhong Peichen	University of California Berkeley	Advancing simulation and learning for complex energy materials From lattice model to CHGNet
I5-07	11:45-12:15	Wang Junjie	Northwestern Polytechnical University	Intelligent Design of Electron-rich Intermetallic Materials
	12:15-13:30	Lunch		

Session Chair: Zhang Dawei, University of Science and Technology Beijing				
I5-08	13:30-14:00	Xiang Xiao-Dong	Southern University of Science and Technology	A Few Key Scientific Issues for MGE
I5-09	14:00-14:30	Kedar Hippalgaonkar	Institute of Materials Research and Engineering, Agency for Science Technology and Research Singapore	From AI and Robotics toward Generative Design of Materials
I5-10	14:30-15:00	Zhang Wei	Xi'an Jiaotong University	Multiscale simulations of phase-change memory materials (Awarded Lecture)
I5-11	15:00-15:30	Wang Xiaonan	Tsinghua University	Integrated platforms for intelligent synthesis, characterization and nanofabrication
	15:30-15:45	Tea Break		
Session Chair: Dominik Legut, Technical University of Ostrava				
I5-12	15:45-16:15	Shi Siqi	Shanghai University	Data Quality Determines the Performance of Machine Learning Model for Materials
I5-13	16:15-16:45	Ji Xiao	Huazhong University of Science and Technology	Microscopic Design of Electrode-Electrolyte Interface
I5-14	16:45-17:15	Zhu Bonan	Beijing Institute of Technology	Applications of crystal structure searching in the exploration of new Li-ion battery cathode materials
I5-15	17:15-17:45	Dai Haiwen	Nanyang Technological University	Data-driven Inorganic Materials Discovery with High-throughput Solid State Synthesis

Symposium 6: AI for Material Science — International Track2

Symposium Organizers: Zhang Dawei, University of Science and Technology; Sun Zhimei, Beihang University; Xue Dezhen, Xi'an Jiaotong University; Liu Zhe, Northwestern Polytechnical University; Zhang Peng, Shanghai Jiao Tong University; Feng Qiang, University of Science and Technology; Zhou Xiaoyuan, Chongqing University; Zhang Xiaokun, University of Electronic Science and Technology of China

Date: Dec 7th 2023 (Beijing time, UTC+8) **Venue: Jinyun Hall, 2nd floor, Shancheng International Conference Center, Chongqing**

No.	Time	Speaker	Affiliations	Presentation Title
Session Chair: Xue Dezhen, Xi'an Jiaotong University				
I6-01	8:30-9:00	Chen Xing-Qiu	Institute of Metal Research, CAS	Development and applications of moment tensor machine learning potential
I6-02	9:00-9:30	Duck Young Kim	Center for High Pressure Science and Technology Advanced Research	Materials discovery under extreme conditions: computational prediction followed by experimental synthesis
I6-03	9:30-10:00	Jason Hattrick-Simpers	University of Toronto	Understanding and Mitigating Bias in Autonomous Materials Characterization and Discovery
	10:00-10:15	Tea Break		
Session Chair: Shi Siqi, Shanghai University				
I6-04	10:15-10:45	Leonardo B. Coelho	Université libre de Bruxelles	Pitting corrosion prediction: from data dispersion analysis to ML estimation of descriptors and domain expertise labelling
I6-05	10:45-11:15	Liao Ting	Queensland University of Technology	Coordination Engineering of Nanomaterials for Sustainable Energy
I6-06	11:15-11:45	Daniel M.Packwood	Kyoto University	Machine learning for functional molecular materials and supramolecular assemblies
I6-07	11:45-12:15	Zhang Dawei	University of Science and Technology Beijing	Data-driven materials discovery and prediction for intelligent corrosion control
	12:15-13:30	Lunch		

Session Chair: Wu Liang, Chongqing University				
I6-08	13:30-14:00	Chen Yue	The University of Hong Kong	Thermal conduction in argyrodite compounds and their alloys
I6-09	14:00-14:30	Zhao Lei	China Iron & Steel Research Institute	High Throughput Microwave Heat-treatment and Characterization Technologies
I6-10	14:30-15:00	Dominik Legut	Technical University of Ostrava	From virtual to reality: a practical route to design new materials
I6-11	15:00-15:30	Tan Jibo	Institute of Metal Research, CAS	Research on multi-factors coupled environmental fatigue behavior of nuclear materials (Awarded Lecture)
	15:30-15:45	Tea Break		
Session Chair: Chang Keke, Ningbo Institute of Materials Technology and Engineering, CAS				
I6-12	15:45-16:15	Lu Haichang	Beihang University	Interfacial engineering of the magnetism and spin transport in two-dimensional materials
I6-13	16:15-16:45	Sviatlana Lamaka	Helmholtz-Zentrum Hereon	High-throughput and in silico exploration of corrosion inhibitors for magnesium
I6-14	16:45-17:15	Zhang Hongbin	Technical University of Darmstadt	Inverse Design of Functional Materials
I6-15	17:15-17:45	Huang Pengru	National University of Singapore	Defect design in 2D materials based on high throughput calculations and machine learning

墙报环节 Poster Session

Poster Session Chair: Zhang Lei, University of Science and Technology Beijing; Feng Zongqiang, Chongqing University

Date：Dec 5th - 7th 2023 (Beijing time, UTC+8)

Venue：Outside Corridor of Changjiang Grand Hall, 1st floor, Shancheng International Conference Center, Chongqing

Online showcase：https://ff04C2R0NP.gctou.top/

No.	Poster Title	Author	Affiliations
P-001	Large-scale Machine-learning Molecular Dynamics Simulation of Primary Radiation Damage in Tungsten	Liu Jiahui	University of Science and Technology Beijing
P-002	Analysis of the Formation Energy Characteristics of Spinel High Entropy Oxides Based On First Principles High Throughput Calculation	Zhou Shengmin	Guilin University of Eletronic Tecnology
P-003	Local Structure and Ageing Property of the Amorphous Ovonic Threshold Switching Material InTe	Wang Huan	Huazhong University of Science and Technology
P-004	Selective Activation of Methane on Hydroxyapatite Surfaces: Insights from Machine Learning and Density Functional Theory	Wang Jing	Sichuan University
P-005	Effects of Rare Earth Oxides Addition on the Corrosion Properties of TiC-based Cermets	Xiao Xuelian	Ningbo Institute of Materials Technology & Engineering, CAS
P-006	Pareto Optimal Driven Automation Framework for Quantitative Microstructure Simulation towards Spinodal Decomposition	Zhang Tongdi	Central South University
P-007	In Search of $Pca2_1$ Phase Ferroelectrics	Mao Geqi	Huazhong University of Science and Technology
P-008	Mechanism of the Effect of Si Content on the High-temperature Oxidation Behaviour of NiAlYSi Alloys Containing Ni5Y Phase	Wang Fangming	Ningbo Institute of Materials Technology & Engineering, CAS
P-009	The Scale Limit and Electron Transport Properties of Ultra-thin Film Phase Change Material $Ge_1Sb_2Te_4$: a DFT-NEGF Study	Wang Bing	Beihang University
P-010	First-principles Calculations Combined with Friction Models to Predict the Moiré Pattern Effect on the Interlayer Friction of Two-dimensional Materials	Zhang Xingwang	Northwestern Polytechnical University
P-011	Design of High-Strength Heat-Resistant Aluminum Alloys Based on Phase Diagram Calculations	Deng Zixuan	Central South University

P-012	Ferroelectricity in 2D Bilayers and Multilayers $MgAl_2S_4$	Wu Peiyao	University of Electronic Science and Technology of China
P-013	Active Design of B-C-N Ternary Compounds with High Thermal Conductivity	Rao Yongchao	Shanghai Jiao Tong University
P-014	Enhanced Crystal Structure Prediction Using Computational and Experimental Data: A Combination of Deep Learning and Optimization Algorithms	Qin Chenglong	Sichuan University
P-015	Doped Sb_2Te_3 Phase Change Materials with Fast Crystallization Speed and High Cycling Endurance Based on Atom Trapping and Pinning Effect	Zeng Yuntao	Huazhong University of Science and Technology
P-016	Research on Ionic Liquid Migration Mechanism and Modulation of Emissivity of Carbon Nanotube Thin Membranes	Wei Xiaoran	National University of Defense Technology
P-017	Aluminum Alloy by Design via Computational Thermodynamics and Machine Learning Techniques	Yi Wang	Central South University
P-018	Research on Overlapping Cascade of Tungsten-based High-entropy Alloys	Wei Guanying	Zhengzhou University
P-019	Molecular Dynamics of Self-healing Behaviour Based on High Entropy Oxides	Liang Jiaqi	Guilin University of Electrical Technology
P-020	Molecular Dynamics Simulation of Biphasic Calcium Phosphate Nanoparticles	Zhang Qiao	Sichuan University
P-021	Atomistic Simulation of [100](001) Crack Propagation with Cu Precipitates in α -iron	Yin Jian	Suzhou Nuclear Power Research Institute
P-022	DFT-based Activity and Stability Analysis of Dry Reforming of Methane Over $Ni1/CeO_2$: Key Role of Crystal Plane Effect	Huang Linan	Kunming University of Science and Technology
P-023	The Local Work Function Distribution of Metals in Nanoscale	Zhou Wenjie	University of Science and Technology Beijing
P-024	Characterization and Modeling Studies towards Al_3Ti/Mg Interfaces in Ti-reinforced AZ31 Alloys	Bao Longke	Harbin Institute of Technology
P-025	Shell DFT-1/2 Enable Material Design of InAs/GaSb Superlattice Infrared Detection	Yang Shengxin	Huazhong University of Science and Technology
P-026	Towards Ultralow-power and High-speed Electronics: Tunnel Transistor Based on Single-chain Tellurium	Zhang Weiming	Beihang University
P-027	Quantitative Phase-field Simulation of Pu Oxidation at Low Temperatures	Ma Sa	Central South University

P-028	Spin Transport Properties of Devices Based on Two-dimensional Chromium Chalcogenides	Wu Qihong	Chongqing University of Posts and Telecommunications
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